

Introduction

Quantum rods are materials that have a characteristic of emitting linearly polarized light and they are attracting attention as next-generation display materials based on their characteristics such as high quantum efficiency and color purity, but in order to be used on an actual device scale, they must meet the essential requirement that all rods be arranged in a line. To arrange quantum rods, several methods have been proposed. In particular, photoalignment is a method in which quantum rods are aligned as liquid crystal molecules gain momentum and rotate as light is irradiated on them. It has an advantage of providing flexibility in the local alignment direction through patterning, but has low dispersibility at high concentrations. Accordingly, we would like to analyze the conditions required for a quantum rod ligand that can be used in photoalignment and propose a structure to improve the degree of quantum rod arrangement.

Result & Discussion

1. Aliphatic vs Aromatic ligand

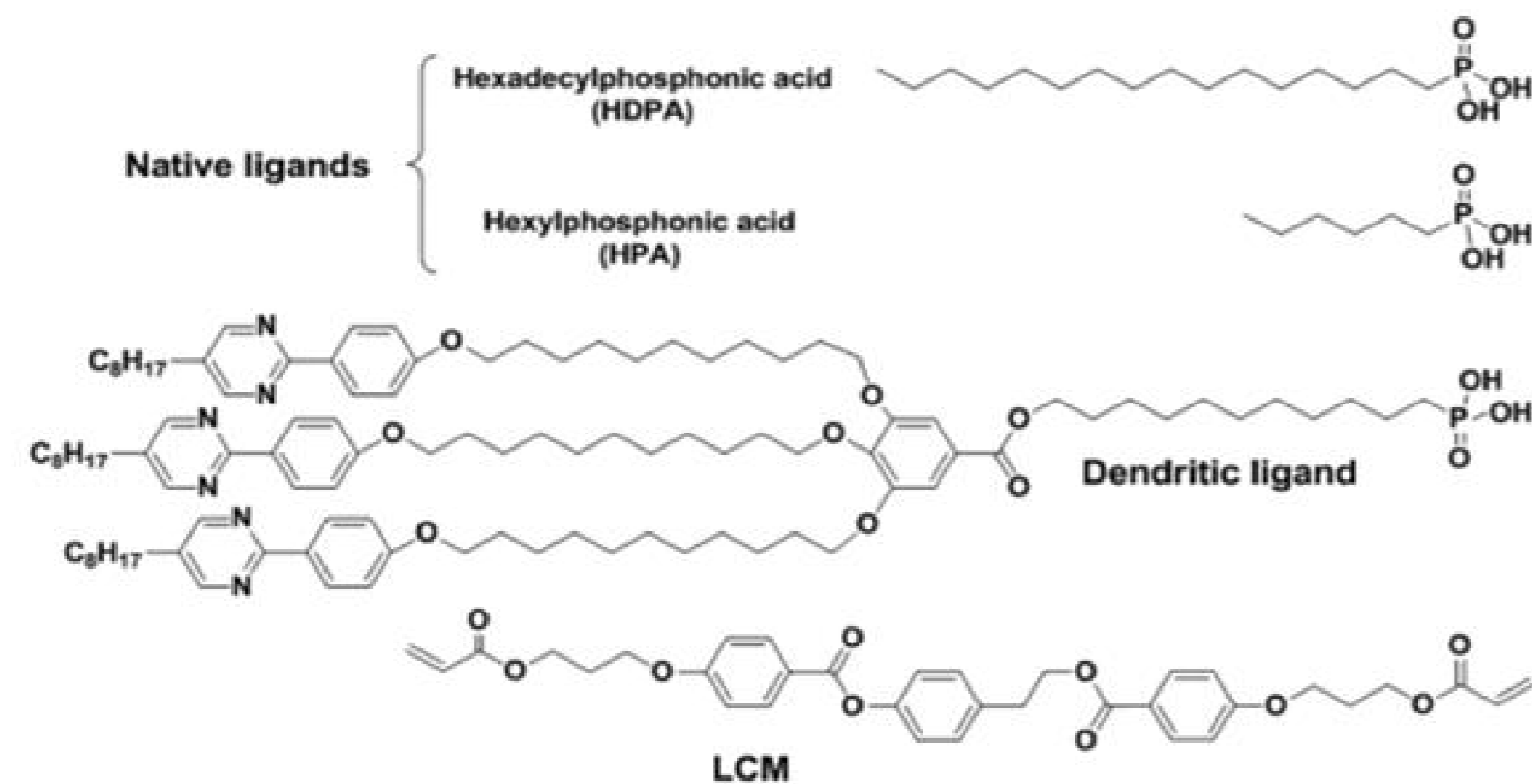


Fig 1. Molecular structures of native ligands, aromatic ligand, and LCM(Liquid crystal monomer)

Since HDPA and HPA are aliphatic ligands and only London displacement forces interact between them, the interaction between them and LCM is poor. Ligands containing aromatic rings can interact more with LCM than aliphatic ligands HDPA and HPA by strong dispersion force and π stacking by higher polarization of π electrons.

2. Horizontal vs Vertical alignment

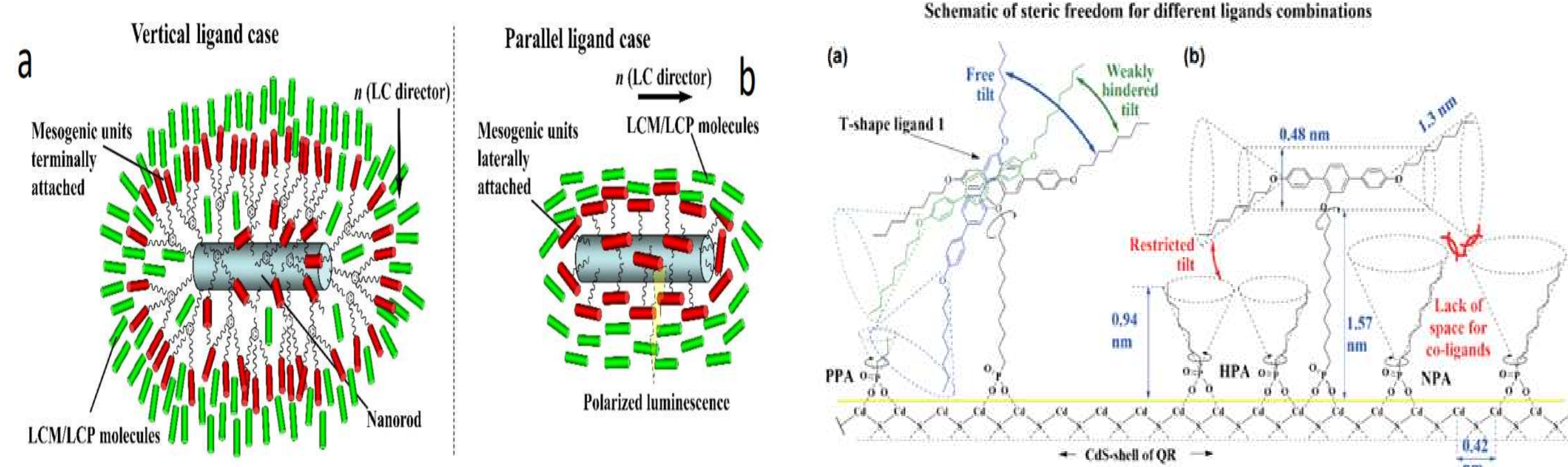


Fig 2. Schematic representation of mutual NR-ligands-LC alignment in case of (a) vertical and (b) parallel ligands;

Fig 3. Illustration of expected ligands alignment on the QR surface for (a) individual TL or TL with a short co-ligand: propylphosphonic acid; (b) TL, diluted with longer co-ligands: hexyl- and nonylphosphonic acid.

When the promesogenic ligand core is attached perpendicularly to the quantum rod, an issue arises where the quantum rod and liquid crystal molecules align perpendicularly, resulting in a decrease in alignment quality as the concentration of quantum rods increases. However, designing the ligand in a T-shaped configuration to horizontally align the quantum rod and ligand core can resolve this problem.

To immobilize the promesogenic core of this T-shaped ligand parallel to the surface of the quantum rod, it is crucial to prevent the core from tilting. Therefore, in addition to the T-shaped ligand, a co-ligand was utilized for this purpose. The alkyl chains of each ligand form a rotation circle due to the absence of rotational energy barriers around the C-C bond. By selecting an appropriate co-ligand, steric hindrance prevents the tilt of the ligands on the quantum rod, ensuring that the promesogenic core is fixed parallel to the quantum rod surface.

3. The length of the co-ligand

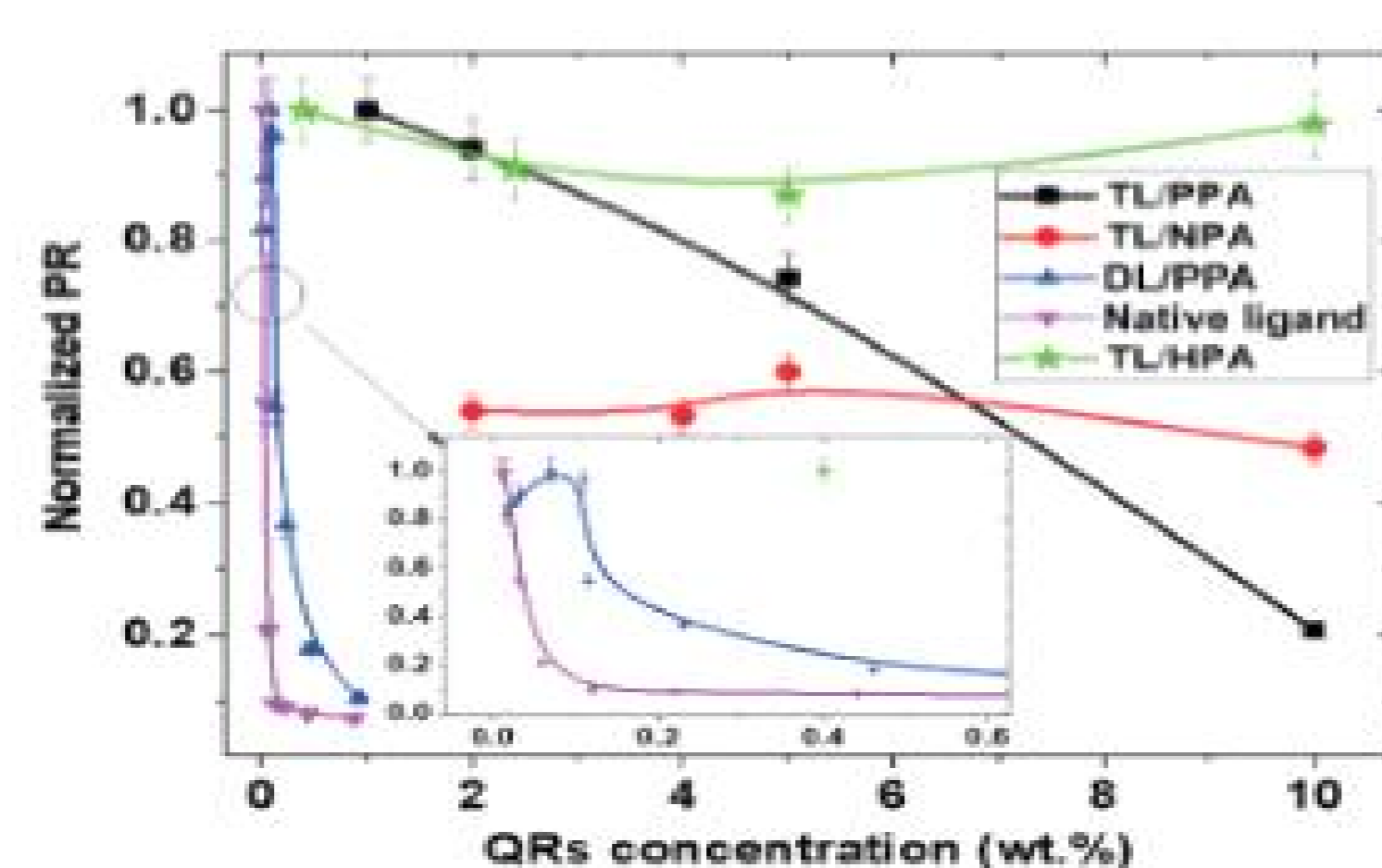


Fig 4. Graph changing the length of the co-ligand

When using a PPA as a co-ligand with a shorter length than HPA, at lower quantum rod concentrations, it exhibits a similar trend to using HPA. However,

as the quantum rod concentration increases, there's a significant decrease in polarization ratio. The portion of the promesogenic cores may rotate, and this causes a tilt along the long axis of the liquid crystal. When employing an NPA longer than HPA as a co-ligand, it yields consistently low polarization ratios regardless of the quantum rod concentration.

In conclusion, quantum rods with an optimal combination of ligands that prevent the tilt of the T-shaped ligand's promesogenic core can effectively align parallel to the liquid crystal.

4. Ligand spacing

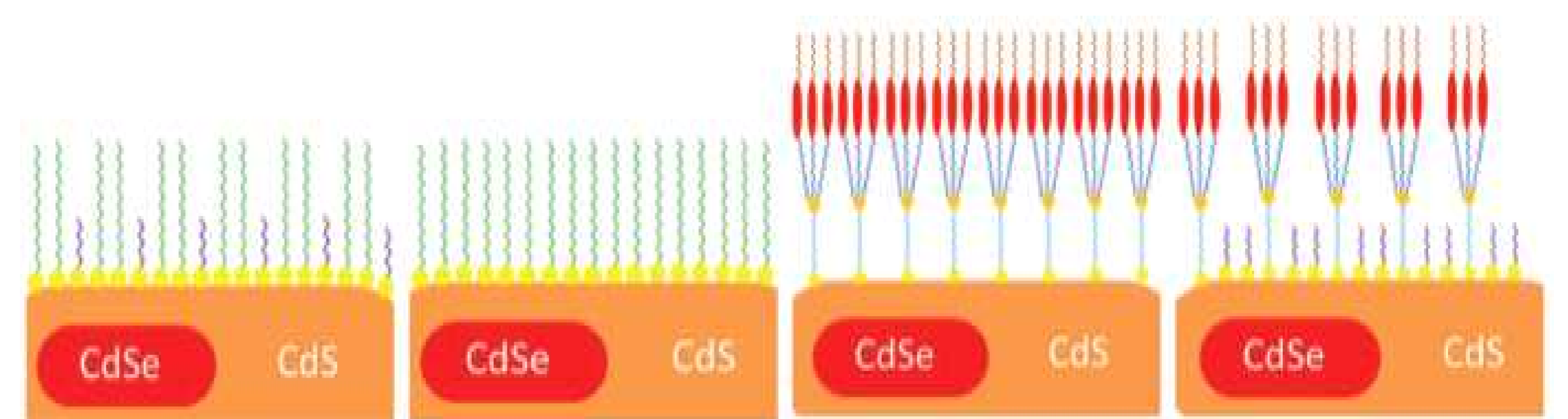
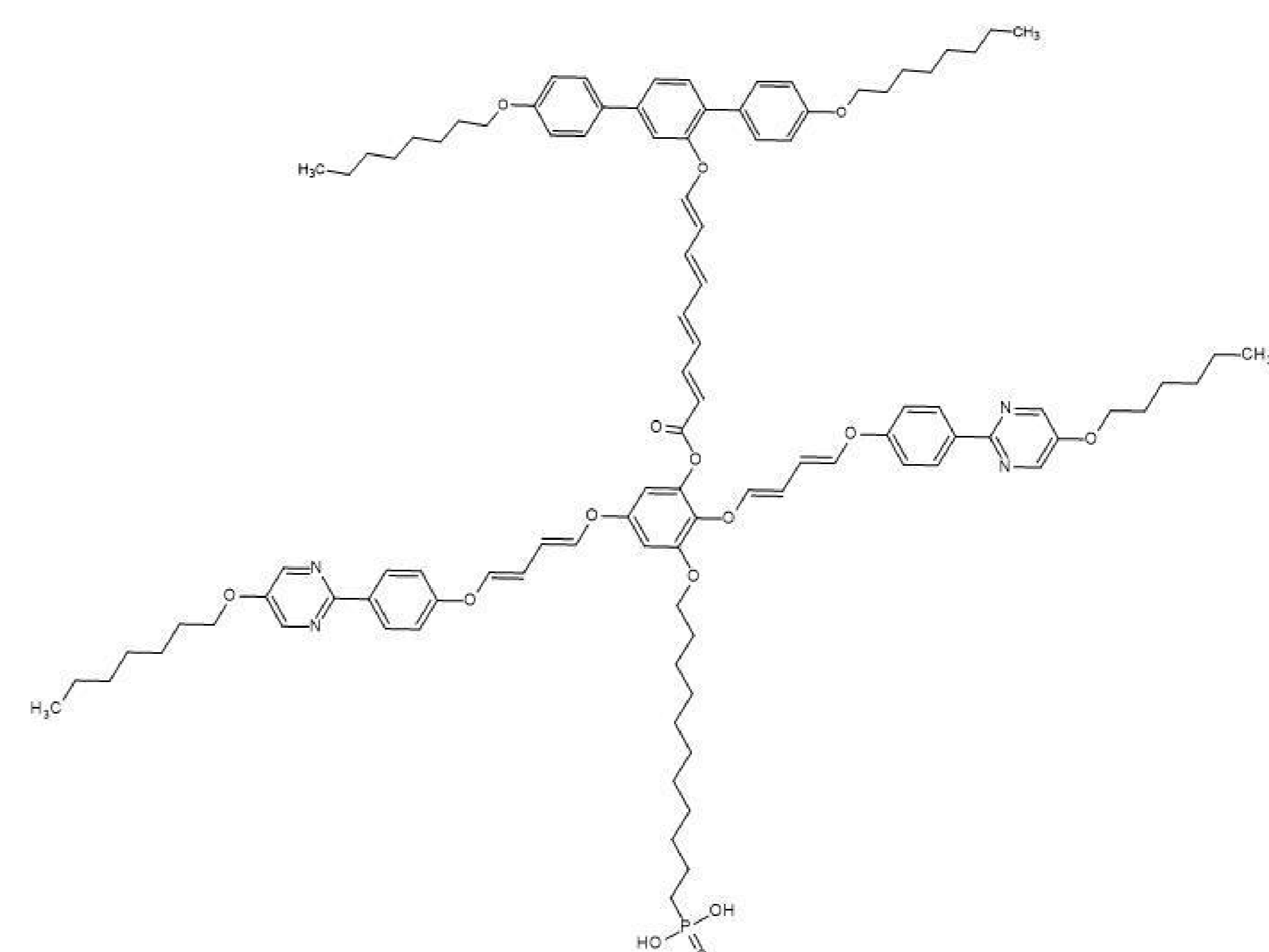


Fig 5. From left to right, adjustment of spacing through combination of HDPA and HPA, individual HDPA, individual dendritic ligands, and the combination of dendritic ligands and HPA to adjust the spacing

When the freedom degree is low, ligands tend to interact strongly with each other and have difficulty interacting with external liquid crystals. Through space adjustment, attaching ligands of various spacers might reduce the penalty even further.

5. Structure suggestion



Characteristics of structure

- Aromatic ligand
- High electron density
- Extended ligand length
- Horizontal alignment

Fig 6. Ligand structure proposed by comprehensively considering the previous contents

Conclusion

In summary, to enhance the alignment of liquid crystal and quantum rods, we proposed a new ligand structure by considering various interactions among quantum rods, ligands, and Liquid Crystal Monomer(LCM). The ligand is designed to induce parallel alignment between quantum rods and LCM. By incorporating stronger aromatic characteristics, we aimed to increase the interaction between the ligand and LCM. Additionally, we carefully considered the space occupied by the ligands and LCM when designing the overall ligand structure. We anticipate that our designed ligand structure will improve the degree of quantum rod arrangement, contributing to the development of LCDs with higher efficiency through enhanced polarization efficiency in quantum rod films.

Reference

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